Nonextensive Thermostatistics and the H-Theorem Revisited

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Abstract

In this paper we present a new derivation of the H-theorem and the corresponding collisional equilibrium velocity distributions, within the framework of Tsallis' nonextensive thermostatistics. Unlike previous works, in our derivation we do not assume any modification on the functional form of Boltzmann's original "molecular chaos hypothesis". Rather, we explicitly introduce into the collision scenario, the existence of statistical dependence between the molecules before the collision has taken place, through a conditional distribution $f(\vec{v}_2|\vec{v}_1)$. In this approach, different equilibrium scenarios emerge depending on the value of the nonextensive entropic parameter.

Boltzmann's kinetic theory, certainly one of the most important developments in the history of statistical mechanics, has as one of its key ingredients the "molecular chaos hypothesis", the celebrated (and somewhat controversial) *Stosszahlansatz*. The irreversible nature of Boltzmann's equation is directly linked to this hypothesis, since molecules in a dilute gas are assumed to be correlated only *after* the collision has taken place [1].

Recently, Lima et al. [2] (see also [3]) advanced an *ad-hoc* modification of the *Stosszahlansatz*, in order to derive a proof of the H-theorem, and to obtain the corresponding collisional equilibrium velocity distribution, within the framework of Tsallis' nonextensive thermostatistics [4]. In this paper, we show that there is no need of modifying the functional form of the molecular chaos hypothesis for accomplishing this task. All we need, besides adopting Tsallis' prescription for the functional form of the local entropy, is to explicitly assume that molecules are also correlated *before* the collision. In other words, we assume that the joint distribution $f(1,2)$ associated with two colliding

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molecules, factorizes as $f(1,2) = f_{1,2} = f(1)f(2|1) = f_1 f_{21}$, where f_{21} contains *all* the information regarding the correlations between 1 and 2, before the impact.

Let us start considering a spatially homogeneous gas of N hard-sphere particles of mass m and diameter s, in the absence of an external force. The state of a dilute gas is kinetically characterized by the velocity distribution function $f(\vec{v}, t)$. The quantity $f(\vec{v}_1, \vec{v}_2, t) d^3 \vec{v}_1 d^3 \vec{v}_2$ gives, at each time t, the number of particles in the volume element $d^3 \vec{v}_1$ around the velocity $\vec{v}_1$ *and* in the volume element $d^3 \vec{v}_2$ around the velocity $\vec{v}_2$. The rate of change of $f(\vec{v}_1, \vec{v}_2, t) d^3 \vec{v}_1 d^3 \vec{v}_2$ verifies the generalized Boltzmann equation

$$\frac{\partial f_{1,2}}{\partial t} = C_q(f_{1,2}) \ , \tag{1}$$

where C_q denotes the generalized collisional term. We also make the usual assumptions: (i) Only binary collisions occur in the gas; (ii) $C_q(f)$ is a local function of the slow varying distribution function; (iii) $C_q(f)$ is consistent with the energy, momentum, and particle number conservation laws. Now, following standard lines we define

$$C_q(f_{1,2}) = \frac{s^2}{2} \int |\vec{V} \cdot \vec{e}| R_q \, d\omega d^3 \vec{v'}_1 d^3 \vec{v'}_2 \ , \tag{2}$$

where the primes indicate post collision quantities, $\vec{V} = \vec{v}_2 - \vec{v}_1$ is the relative velocity before collision, $\vec{e}$ denotes an arbitrary unit vector, and $d\omega$ is an elementary solid angle such that $s^2 d\omega$ is the area of the collision cylinder [5,6]. The quantity $R_q(f, f')$ is a difference of two correlation functions (just before and after collision). At this point we depart from [2], who originally proposed that $R_q(f, f') = \exp_q(f_1'^{q-1} \ln_q f_1') + f_2'^{q-1} \ln_q f_2') - \exp_q(f_1^{q-1} \ln_q f_1) + f_2^{q-1} \ln_q f_2)$, where $\exp_q$ and $\ln_q$ are q-exponential and q-logarithmic functions (see below), and assume that $R_q(f, f')$ simply satisfies the *standard* functional form of Boltzmann's molecular chaos hypothesis

$$R_q(f, f') = f_1' f_{21}' - f_1 f_{21} \ , \tag{3}$$

where again primes refer to the distribution function after collision. Note that, although the functional form is the same, there is a subtle but profound difference between ours and Boltzmann's original approach, in the sense that now velocities of colliding molecules are *not* statistically independent before the impact.

For the joint entropy we adopt Tsallis' expression,

$$H_q^{1,2} = -k \int f_{1,2}^q \ln_q f_{1,2} \, d^3 \vec{v}_1 d^3 \vec{v}_2 \ , \tag{4}$$

where $\ln_q = \frac{f^{1-q}-1}{1-q}$. Note that $H_q^{1,2}$ reduces to the standard Boltzmann extensive measure $H^{1,2} = H^1 + H^2$, for $q = 1$. Taking the partial time derivative of the above expression we obtain

$$\frac{\partial H_q^{1,2}}{\partial t} = -k \int (q f_{1,2}^{q-1} \ln_q f_{1,2} + 1) \frac{\partial f_{1,2}}{\partial t} \, d^3\vec{v}_1 d^3\vec{v}_2 \quad . \tag{5}$$

Inserting the generalized Boltzmann equation (1) into (5), and using (2), expression (5) can be rewritten as a balance equation

$$\frac{\partial H_q^{1,2}}{\partial t} = G_q(t) \quad , \tag{6}$$

where the source term G_q reads

$$G_q = -\frac{ks^2}{2} \int |\vec{V} \cdot \vec{e}|(1 + q f_{1,2}^{q-1} \ln_q f_{1,2}) R_q \, d\omega d^3\vec{v}_1 d^3\vec{v}_2 d^3\vec{v'}_1 d^3\vec{v'}_2 \quad . \tag{7}$$

In order to rewrite G_q in a more symmetrical form, some elementary operations must be done in the above expression. Following standard lines [5], we first notice that interchanging $\vec{v}_1$ and $\vec{v}_2$ does not affect the value of the integral. This happens because the magnitude of the relative velocity vector and the scattering cross section are invariants. Similarly, we may use time-reversal symmetry. Note that this step requires the change of sign of R_q (inverse collision). Implementing these operations and symmetrizing the resulting expression, one may show that the source term can be written as

$$G_q = -\frac{ks^2}{4} \int |\vec{V} \cdot \vec{e}|(q f_{1,2}^{q-1} \ln_q f_{1,2} - q f_{1,2}'^{q-1} \ln_q f_{1,2}')$$
$$R_q \, d\omega d^3\vec{v}_1 d^3\vec{v}_2 d^3\vec{v'}_1 d^3\vec{v'}_2 \quad . \tag{8}$$

Noting that $f_{1,2} = f_1 f_{21}$, and applying the transformation $f^{q-1} \ln_q f = \ln_{q^*} f$, where $q^* = 2 - q$, we finally find

$$G_q = \frac{ks^2 q}{4} \int |\vec{V} \cdot \vec{e}|(\ln_{q^*}(f_1' f_{21}') - \ln_{q^*}(f_1 f_{21}))(f_1' f_{21}' - f_1 f_{21})$$
$$d\omega d^3\vec{v}_1 d^3\vec{v}_2 d^3\vec{v'}_1 d^3\vec{v'}_2 \quad . \tag{9}$$

For positive values of q, the q-log function is concave. Thus, the integrand in equation (9) is never negative because $(\ln_{q^*} f_1' f_{21}' - \ln_{q^*} f_1 f_{21})$ and $(f_1' f_{21}' - f_1 f_{21})$

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always have the same sign. Therefore, we obtain the H_q-theorem

$$\frac{\partial H_q^{1,2}}{\partial t} \geq 0 \quad , \tag{10}$$

for $q^* > 0$ or, equivalently, $0 < q < 2$. This inequality describes the route to equilibrium within the framework of Tsallis' nonextensive formalism. We remark that, since f_1 and f_2 are not statistically independent, we cannot say anything about H_q^1 (or H_q^2) individually, whose value may even decrease during the relaxation process.

Now, to obtain the equilibrium q-distribution all we need is to set $G_q = 0$. Since the integrand appearing in (9) cannot be negative, the source term will vanish, for any pair of molecules obeying the energy, momentum, and particle number conservation laws, if and only if

$$f_1' f_{21}' = f_1 f_{21} \quad , \tag{11}$$

or equivalently

$$\ln_q f_1' + \ln_q f_{21}' + (1-q) \ln_q f_1' \ln_q f_{21}' = \ln_q f_1 + \ln_q f_{21} + \\ (1-q) \ln_q f_1 \ln_q f_{21} \quad . \tag{12}$$

Clearly, $\ln_q f_1$ and $\ln_q f_{21} + (1-q) \ln_q f_1 \ln_q f_{21}$ are collision invariants. Thus, the marginal equilibrium distribution must be of the form

$$\ln_q f_1 = a_0 + \vec{a}_1 \cdot \vec{v}_1 + a_2 \vec{v}_1 \cdot \vec{v}_1 \quad , \tag{13}$$

where a_0 and a_2 are constants and $\vec{a}_1$ is an arbitrary constant vector. By introducing the barycentric velocity $\vec{u}$, we may rewrite (13) as

$$\ln_q f_1 = \alpha - \gamma |\vec{v}_1 - \vec{u}|^2 \quad , \tag{14}$$

with a different set of constants. Now, defining $\Gamma_q = e_q(\alpha)$ and $\beta = \frac{\gamma}{(1+(1-q)\alpha)}$, we obtain a q-generalized Maxwell's distribution

$$f_0(\vec{v}_1) = \Gamma_q \, e_q(-\beta|\vec{v}_1 - \vec{u}|^2) = \Gamma_q \, [1 - (1-q)\beta|\vec{v}_1 - \vec{u}|^2]^{1/1-q} \quad , \tag{15}$$

where $e_q(x) = [1 + (1-q)x]^{1/1-q}$, and Γ_q, β and $\vec{u}$ may be functions of the temperature. This result is identical to that obtained in Ref. [2], using a very

different functional form for the molecular chaos hypothesis. Naturally, Boltzmann's classical scenario, and its corresponding results, are recovered in the limit of $q \to 1$.

Now, assuming that, by collision invariance, we have in equilibrium $\ln_q f_{21} + (1-q)\ln_q f_1 \ln_q f_{21} \sim -\beta(|\vec{v}_2 - \vec{u}|^2)$, the q-generalized conditional and joint distributions can be easily obtained

$$f_0(\vec{v}_2|\vec{v}_1) = \Lambda_q \, e_q \left(\frac{-\beta|\vec{v}_2 - \vec{u}|^2}{1 - (1-q)\beta|\vec{v}_1 - \vec{u}|^2} \right) \quad , \tag{16}$$

and

$$f_0(\vec{v}_1, \vec{v}_2) = \Theta_q \, e_q[-\beta(|\vec{v}_1 - \vec{u}|^2 + |\vec{v}_2 - \vec{u}|^2)] \quad , \tag{17}$$

with Θ_q and Λ_q being the appropriate normalization factors.

Note that, although $\vec{v}_1$ and $\vec{v}_2$ are, by definition, statistically *dependent*, is easy to verify that the covariance $\langle \vec{v}_1, \vec{v}_2 \rangle$ equals zero, regardless the value of q. A natural question arises from this somewhat paradoxycal result: what is therefore the effect induced by nonextensivity on the classical picture of a dilute gas?

To answer this question we plotted in Fig. 1 the function $\chi_q(\vec{v}_1, \vec{v}_2)$, where $f_{1,2} = \chi_q f_1 f_2$, for three values of the entropic parameter. χ_q acts as a q-generalized, velocity-dependent Enskog factor, reducing or enhancing the collision frequency at certain velocities. For $q > 1$, high-velocity collisions are favored, the *rms* velocity increases, the mean collision time decreases, and the velocity distribution ceases to be a Gaussian, displaying power-law tails. Strong, intermittent fluctuations on the velocity and the particle density fields are expected to emerge. This behavior is reminiscent to that observed in granular gases [7]. For $q < 1$, we have the opposite scenario: high-velocity collisions are filtered, the *rms* velocity decreases, the mean collision time increases, and the velocity distribution displays a cut-off, meaning that the gas occupies only a subset of its phase space. A condensate of cold, motionless particles may eventually appear. Naturally, for $q = 1$, we have $\chi_q = 1$, regardless the velocities, what recovers Boltzmann's original molecular chaos hypothesis.

Summarizing, in this paper we presented a new derivation of the H-theorem and the corresponding collisional equilibrium velocity distributions, within the framework of Tsallis' nonextensive thermostatistics. Unlike previous works, in our derivation we do not assume any modification on the functional form of Boltzmann's original "molecular chaos hypothesis". Rather, we explicitly introduced into the collision scenario, the existence of statistical dependence between the molecules before the collision, through a conditional distribution
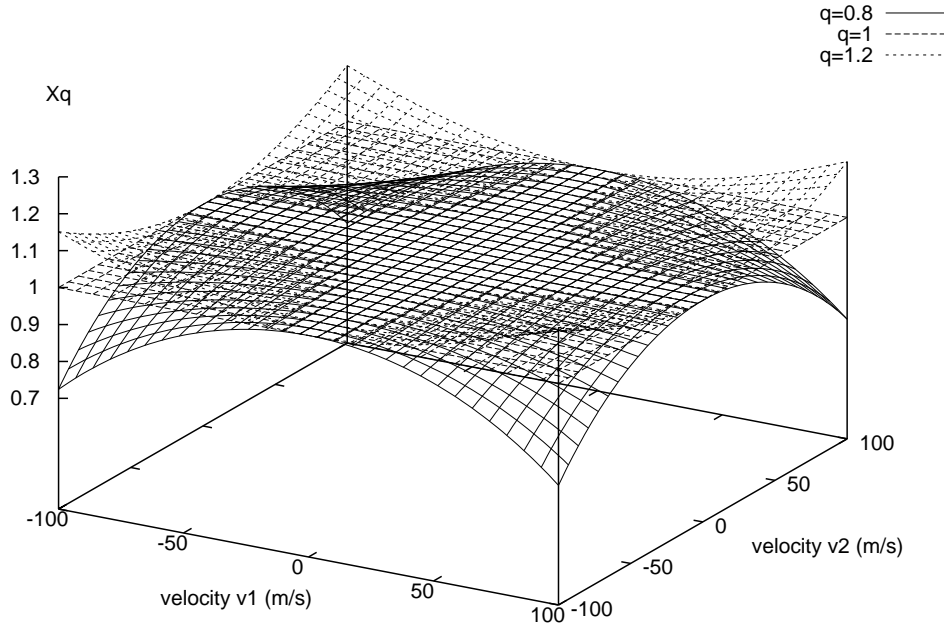
Fig. 1. Variation of χ_q for $q = 1.2$ (top), $q = 1$ (intermediate) and $q = 0.8$ (bottom).

$f(\vec{v}_2|\vec{v}_1)$. In this approach, different equilibrium scenarios emerge depending on the value of the nonextensive parameter.

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